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ABSTRACT

We present a preliminary investigation of damage localization as a model problem for adaptive sampling. The fine-scale material response involving void nucleation and growth is computed on the fly as needed at the coarse scale.

1 Adaptive Sampling of Fine-scale Physics

The construction of multiscale models is quite diverse, ranging from sequential approaches to concurrent methodologies [1]. Here we are particularly interested in the class of systems where the entirety of the state space at the fine scale(s) is too vast to permit pre-computation of the material response, but the scales are well separated and the fine-scale evolution only depends on the coarse-scale state locally. Then it is possible to envisage a methodology that computes the fine-scale material behavior on the fly, as it is needed by the coarse-scale simulation. For example, the fine-scale behavior may depend strongly on the initial microstructure and how it evolves under deformation. Both the initial configuration space and the possible histories may be vast and impossible to pre-compute. Nevertheless, it might be possible to compute a homogenized response such as a plastic strain increment for a given microstructure on the fly. Typically the fine-scale calculations are expensive computationally, so the challenge is to formulate an intelligent approach that allows the coarse-scale calculation to be completed at the desired level of accuracy with the minimal amount of fine-scale calculation. The key to the success of such an *adaptive sampling* approach is to minimize redundant or superfluous fine-scale calculations.

The application of interest here is damage localization. At the coarse scale the material deformation results from plastic flow in response to shear stresses and plastic dilation due to the increasing porosity. At the fine scale this porosity is resolved into voids that nucleate from second phase particles, grow and coalesce leading to material failure. We are interested in how the random distribution of void nucleation thresholds (related to the inclusion size distribution, etc.) and local heating affect the degree to which the deformation is localized in damage bands.

2 Numerical Methods

At the coarse scale we have a one-dimensional system (a beam) taken to be a viscous solid in expansion in the longitudinal direction. The system is taken to be periodic in the longitudinal direction, and elongated at a linearly increasing strain rate. The viscous response of the solid is given by $\sigma = \alpha(\dot{\varepsilon}_v)^n$ where σ is the stress and α and n are material constants. The viscous strain rate, $\dot{\varepsilon}_v$, is given by the difference between

the total strain rate and the rate of porosity increase $\dot{\varepsilon}_v = \dot{\varepsilon} - \dot{p}$ where $\dot{\varepsilon}$ is the total strain rate and p is the porosity. The dots denote time derivatives. The porosity is computed on the fly by a fine-scale model. Thermal conduction is also computed. The local temperature affects the development of porosity which in turn causes heating.

Ultimately, a sophisticated and expensive model of void growth will be used at the fine scale, but for the purposes of this preliminary work, the void growth is described by a DFRACT model [2]: $\dot{p}_i = p_i(\sigma - \sigma_0)/\nu$, where p_i is the volume fraction of the i^{th} void, σ is the mean (hydrostatic) stress, σ_0 is the mean stress threshold for growth, and ν is the viscosity. Void nucleation takes place at a mean tensile stress and void volume drawn from Gaussian distributions. These distributions are calculated at the beginning of the simulation, so the initial microstructure is completely specified. The input for the fine-scale model is the local stress and temperature, and the resulting output is the rate of porosity increase. We have found that it is necessary to compute the porosity rate implicitly in order to achieve numerical stability.

A coupling code provides an interface between the coarse-scale and fine-scale models, and it controls the adaptive sampling. In practice, just like the fine-scale model, its role is to provide the data $\dot{p}[\sigma(x,t), T(x,t); x]$ to the coarse-scale model. At each point, the coarse-scale model provides the temperature $T(x)$ and the stress $\sigma(x)$, and the coupling routine returns the rate of porosity increase. The coupling model appears to the coarse-scale code to be a material response database. This kind of interface is important for minimally invasive implementation of on-the-fly multiscale modeling. In practice it does one of two things. Based on a sampling criterion that incorporates knowledge of the finite temperature threshold, the coupling model either returns a database value for $\dot{p}$ where available or it queries (or spawns and queries) a fine-scale simulation to determine $\dot{p}$, and returns that value.

3 Results and Discussion

We have used the adaptive sampling algorithm described above to investigate the development of localized fracture with a particular interest in the effective speed up that can be obtained and how it depends on the degree to which the damage is localized. The results of two simulations are shown in Fig. 1. The porosity is plotted as a function of position in the one-dimensional system. The coarse-scale model consisted of 1000 finite elements with linear shape functions and single point quadrature. Each element contained 100 void nucleation sites with normally distributed random nucleation thresholds whose standard deviation was 20% of the mean. Failure occurred when the porosity in any one element reached 0.1. The difference in the two simulations was the temperature dependence of the void growth threshold. The system with a greater temperature dependence tended to localize the damage to one or a few elements, as the heat generated by the initial void growth promoted further void growth. The onset of this damage localization instability could also be triggered by changes in the strain rate, nucleation threshold distribution and growth viscosity.

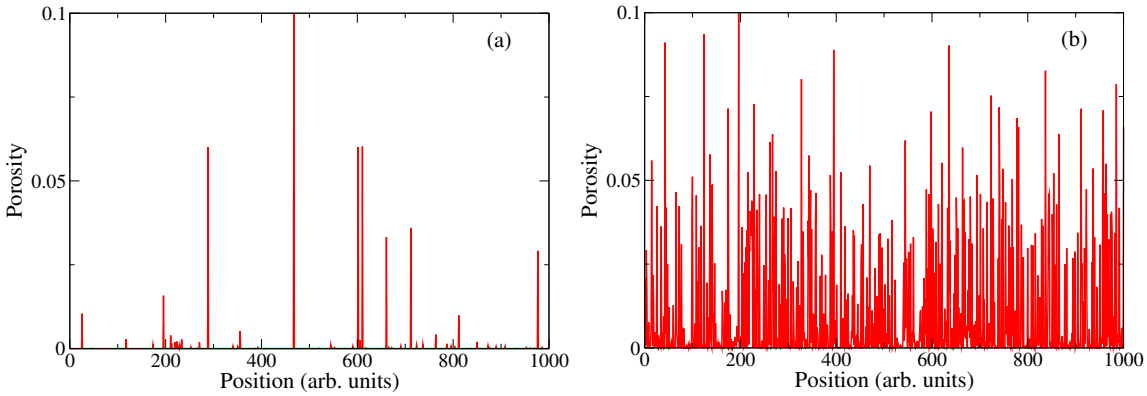

Figure 1: Porosity at failure due to void growth from a random distribution of nuclei: (a) greater damage localization due to heating and (b) negligible heating.

While these preliminary simulations were done with a fairly inexpensive void growth model, our goal is to use high fidelity fine-scale calculations including molecular dynamics. Then the fine-scale calculations will dominate the computational cost, and so we quantify the speed up as the ratio of the total number of material model calls in the coarse-scale elements to the number that involve a fine-scale calculation (a ratio of 1 indicates no speed up). The main result, for our purposes here, is that by adjusting the parameters of the model we have attained different levels of damage localization and quantified the speed up due to the adaptive sampling approach. In the highly localized case (Fig. 1a), the ratio of the total number of material model calls in the coarse-scale elements to the number that involve a fine-scale calculation was 203 and a total of 180 voids nucleated; in the poorly localized case (Fig. 1b), the sampling ratio was 26 and a total of 4282 voids nucleated.

These simple toy model calculations indicate that adaptive sampling may be used quite effectively in order to speed up multiscale simulations relying on on-the-fly calculation of fine-scale material response. The proof, of course, will lie in the implementation of this algorithm in more realistic simulations. As a by-product, the simple model indicates that damage localization may exhibit a rich physical phenomenology as thermal and mechanical materials properties are varied.

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